

# Lattice Simulations of the Quantum Microcanonical Ensemble

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We propose a method for the numerical computation of microcanonical expectation values—i.e. averages over energy eigenstates with the same eigenvalue—without any prior knowledge about the spectrum of the Hamiltonian. This is accomplished by first defining a new Gaussian ensemble to approximate the microcanonical one. We then develop a “lattice theory” for this Gaussian ensemble and propose a Monte Carlo integration of the expectation values of the lattice theory.

## I. INTRODUCTION

The microcanonical ensemble is considered to be the fundamental ensemble of statistical physics. For example, the use of the canonical Gibbs ensemble is usually justified by showing that its expectation values coincide with the microcanonical ones in the infinite-volume limit. However, since an application of the microcanonical ensemble requires detailed knowledge about the energy levels of the system, it is seldom possible to use it in practice. The canonical ensemble, on the other hand, has a well-behaved path-integral expression easily extended to the gauge field theories—therefore it has become the standard ensemble of quantum statistics.

Nevertheless, there are situations where the easiest alternative does not work. For instance, direct applications of the grand canonical ensemble have not been able to reproduce all the results of the relativistic ion collision experiments.<sup>1</sup> There are two possible explanations for this shortcoming of the canonical ensemble: either the particle gas created in the collision does not reach thermal equilibrium before exploding into the final state hadrons, or the system is too small to be handled by the canonical methods.

Recent calculations<sup>2</sup> using the grand canonical ensemble with finite-volume corrections have, however, succeeded in describing most of the particle abundances in heavy ion collisions. This suggests that at least the final state hadron gas will thermalize, but it also shows that the finite-volume effects are prominent in these systems.

These results point into the direction that the microcanonical ensemble—which is optimal for describing isolated ergodic systems with small quantum numbers—should be used for getting quantitative information about the properties of the quark-gluon plasma possibly created in the relativistic hadron collisions. The continuum path integral formulation of the microcanonical ensemble and the corresponding perturbation theory have already been developed both for scalar<sup>3</sup> and gauge field theories,<sup>4</sup> but since the phenomena involving hadrons happen in the low energy, strong coupling regime, non-perturbative methods are

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also needed. However, no general numerical treatment is presently available to compute microcanonical expectation values without *a priori* knowledge about the energy spectrum even in the quantum mechanical context, let alone in a quantum field theory. In this paper, we aim at a development of such a method in the spirit of lattice field theories for a class of quantum mechanical Hamiltonians. The generalization of these results to the more interesting case of gauge field theories, such as quantum chromodynamics, is a subject of further work.

The paper is divided into three parts: the first section introduces a new statistical ensemble, called a Gaussian ensemble, and establishes its close connection to the microcanonical one. In the second section we will derive lattice integral kernels for a numerical evaluation of the Gaussian expectation values. Due to the complicated nature of these kernels, it is not immediately evident how Monte Carlo methods can be used in this computation—this will be the subject of the rest of the paper.

## II. THE GAUSSIAN ENSEMBLE<sup>5</sup>

Consider the operator defined by

$$\hat{\rho}_\varepsilon(E) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left[-\frac{1}{2} \left(\frac{\hat{H} - E}{\varepsilon}\right)^2\right], \quad (1)$$

where  $\hat{H}$  is the Hamiltonian. This operator is clearly bounded, self-adjoint and positive. Let us assume that the spectrum of the Hamiltonian is discrete with eigenvalues  $E_n$ , each of which has a finite number of eigenvectors  $\Omega_{n,k}$ ,  $k = 1, \dots, \kappa_n$ , where  $\kappa_n$  is the multiplicity of the eigenvalue  $E_n$ . With rather loose assumptions on the eigenvalues ( $\lim_{n \rightarrow \infty} n^s/E_n = 0$  for some  $s > 0$ ) will suffice if the multiplicities  $\kappa_n$  diverge at most polynomially in  $n$ )  $\hat{\rho}_\varepsilon$  is trace-class and therefore defines a sensible statistical ensemble via

$$\langle \hat{A} \rangle \equiv \frac{\text{Tr}(\hat{\rho}_\varepsilon \hat{A})}{\text{Tr} \hat{\rho}_\varepsilon}, \text{ for any observable } \hat{A}. \quad (2)$$

Note that if the Gibbs ensemble is well-defined for temperature  $2\varepsilon^2$ , i.e.  $\text{Tr} \exp(-\frac{1}{2\varepsilon^2} \hat{H}) < \infty$ , then  $E_n - E < 1$  only for finitely many  $n, k$  and, since for the rest  $(E_n - E)^2 \geq E_n - E$ ,  $\hat{\rho}_\varepsilon(E)$  is then trace-class. This means that the Gaussian ensemble is well-defined for all systems for which we can use the canonical one.

Intuitively, the above density operator describes a system that was initially prepared into a Gaussian energy distribution  $E \pm \varepsilon$ , but which has then stabilized under ergodic evolution in isolation. This, with the formal relation  $\lim_{\varepsilon \rightarrow 0} \hat{\rho}_\varepsilon(E) = \delta(\hat{H} - E)$ , will give the physical motivation for using this ensemble to approximate the microcanonical one. However, it can also be argued that the Gaussian ensemble is even better suited for describing real experimental situations than the microcanonical ensemble, since it naturally incorporates the energy resolution of the experiment through the parameter  $\varepsilon$ —in any real experiment the total energy of the system (e.g. of a particle) cannot be known exactly, but only within a certain accuracy. We will now turn to the mathematical justification of these formal statements.

Using the earlier notations, we can express the trace in (2) as

$$\text{Tr}(\hat{\rho}_\varepsilon \hat{A}) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \sum_{n,k} \exp\left[-\frac{1}{2\varepsilon^2} (E_n - E)^2\right] \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle. \quad (3)$$

Since

$$\lim_{\varepsilon \rightarrow 0} \exp\left[-\frac{1}{2\varepsilon^2} (E_n - E)^2\right] = 0, \text{ when } E \neq E_n, \quad (4)$$

the partition function clearly satisfies

$$\lim_{\varepsilon \rightarrow 0} \text{Tr} \hat{\rho}_\varepsilon = \sum_n \kappa_n \delta(E - E_n) = Z_{\text{microcan}}. \quad (5)$$

In the evaluation of the limit of the expectation values, we need the result

$$\frac{1}{\sum_{n',k'} \exp\left[-\frac{(E_{n'} - E)^2 - (E_n - E)^2}{2\varepsilon^2}\right]} \longrightarrow \begin{cases} 0, & \text{if } |E_{n'} - E| < |E_n - E| \text{ for some } n' \\ (\sum_{n'} \kappa_{n'} \delta_{|E_{n'} - E|, |E_n - E|})^{-1}, & \text{otherwise} \end{cases}. \quad (6)$$

In other words, this limit is zero if  $E_n$  is not the eigenvalue nearest to  $E$ , it is  $(\kappa_n + \kappa_{n'})^{-1}$  if both  $E_n$  and  $E_{n'}$  are nearest eigenvalues (i.e. if  $E$  lies exactly in the middle of the segment joining  $E_n$  and  $E_{n'}$  and no other eigenvalues are on this segment) and it is  $\kappa_n^{-1}$  if  $E_n$  is a unique nearest eigenvalue. Let us use notation  $M_n(E)$  for the sum  $\sum_{n'} \kappa_{n'} \delta_{|E_{n'} - E|, |E_n - E|}$ .

Using the formula (3) for the traces and (6) to compute the limit, we arrive at

$$\langle \hat{A} \rangle = \sum_{n,k} \frac{\exp\left[-\frac{1}{2\varepsilon^2} (E_n - E)^2\right]}{\text{Tr} \hat{\rho}_\varepsilon \sqrt{2\pi\varepsilon^2}} \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle \longrightarrow \frac{1}{M_{n_0}(E)} \sum_{n,k} \delta_{|E_n - E|, |E_{n_0} - E|} \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle, \quad (7)$$

where  $n_0$  is the index of an eigenvalue nearest to  $E$ . Since  $M_{n_0}(E)$  is the number of terms in the last sum, the last expression is nothing but the average of the expectation values of  $\hat{A}$  over the energy eigenstates nearest to  $E$ .

Therefore, whenever  $E$  coincides with a point in the spectrum, the limit  $\varepsilon \rightarrow 0$  will give the microcanonical expectation value. On the other hand, if  $E$  does not belong to the energy spectrum (in which case the microcanonical ensemble is in principle ill-defined), then the microcanonical result corresponding to the nearest eigenvalue is obtained. The only values of  $E$  giving non-microcanonical limits are those lying exactly in the middle between two eigenvalues, but even then the result is an expectation value of a uniform distribution over two energy eigenvalues.

In the above, we tacitly assumed that it is possible to exchange the order of the limit and the sum over  $n$ . This operation is in fact allowed if the sum in (3) converges absolutely for any  $\varepsilon$ , which for positive  $\hat{A}$  is tantamount to the assumption  $\langle \hat{A} \rangle_\varepsilon < \infty$ . We will now prove this by showing that if (3) converges absolutely for  $\varepsilon_0 > 0$ , then the series in (7) converges uniformly for  $0 < \varepsilon \leq \varepsilon_0$ .

Let  $n_0$  be, as before, the index of one of the eigenvalues nearest to  $E$ . Since  $\exp(-\frac{C}{\varepsilon^2})$  is an increasing function of  $\varepsilon$  for  $C, \varepsilon > 0$ , we immediately see that

$$\frac{1}{\sum_{n',k'} \exp\left[-\frac{(E_{n'} - E)^2 - (E_{n_0} - E)^2}{2\varepsilon^2}\right]} < \exp\left[-\frac{(E_n - E)^2 - (E_{n_0} - E)^2}{2\varepsilon_0^2}\right] \quad (8)$$

for all  $n$  such that  $|E_n - E| > |E_{n_0} - E|$ . In fact, this inequality extends also to the case  $|E_n - E| = |E_{n_0} - E|$ , since the ratio on the left hand side is always less than one. Therefore, the absolute value of each of the terms of the series in (7) is less than  $\exp[(E_{n_0} - E)^2/(2\varepsilon_0^2)] \exp[-(E_n - E)^2/(2\varepsilon_0^2)] |\langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle|$ , which again form an  $\varepsilon$ -independent sum that is convergent by assumption. Thus the series in (7) satisfies the Weierstrass  $M$ -test and is uniformly convergent.

The uniform convergence of  $\sqrt{2\pi\varepsilon^2} \text{Tr } \hat{\rho}_\varepsilon$  is similarly established by the Weierstrass  $M$ -test using the monotonicity of  $\exp[-(E_n - E)^2/(2\varepsilon^2)]$ .

### III. DERIVATION OF THE LATTICE ENSEMBLE

In this section we will derive a “lattice approximation” of the Gaussian ensemble for quantum mechanical Hamiltonians of the type  $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ , where  $V$  is a suitable potential function. For example, if  $V$  were a (non-constant) polynomial bounded from below, then  $\hat{H}$  would be essentially self-adjoint and the operator  $e^{-\beta\hat{H}}$  would be trace-class with the usual Feynman-Kac path-integral kernel. Also, for any polynomial and for all bounded functions  $A$ , the canonical expectation values would then be well-defined and could be computed by using the formula<sup>6,7</sup>

$$\text{Tr} \left[ A(\hat{x}) e^{-\beta\hat{H}} \right] = \lim_{N \rightarrow \infty} \int \frac{d^N x d^N p}{(2\pi)^N} A(x_0) \exp \left[ i \sum_{k=1}^N p_k (x_{k-1} - x_k) - \frac{\beta}{N} \sum_{k=1}^N \left( \frac{p_k^2}{2m} + V(x_k) \right) \right], \quad (9)$$

where  $x_0 = x_N$  and  $\beta > 0$ .

In the following we will need the analytic continuation of this result to the region  $\text{Re } \beta > 0$ . If  $V$  is a second-order polynomial, i.e. if we consider a harmonic oscillator, then this continuation can be computed exactly and it is seen to be given by (9). There is no apparent reason why the same continuation should not work for any polynomial, but we have not yet been able to construct a proof of this generality.<sup>8</sup> We will therefore simply assume that  $V$  is a potential such that (9) holds for all  $\text{Re } \beta > 0$ .

It will be useful to define a few auxiliary quantities for the computation of the lattice expectation values. Firstly, the relevant energy parameter of the lattice Gaussian distribution will turn out to be  $E/\varepsilon$  and we will use a separate notation  $W$  for this dimensionless quantity. Secondly, we will need the following three “action-like” quantities:

$$S_0(x; \varepsilon) = \frac{1}{N\varepsilon} \sum_{k=1}^N \frac{m}{2} \left( \frac{x_{k-1} - x_k}{1/(N\varepsilon)} \right)^2, \quad S_1(x; \varepsilon) = \frac{1}{N\varepsilon} \sum_{k=1}^N V(x_k) \quad (10)$$

and, finally,  $S(p, x; \varepsilon) = \frac{1}{N\varepsilon} \sum_{k=1}^N \frac{p_k^2}{2m} + S_1(x; \varepsilon)$ . A comparison with (9) reveals that  $S$  is nothing but the usual finite-temperature lattice action for temperature  $T = \varepsilon$ .

In order to keep track of all the mathematical details in the derivation of the lattice ensemble, we need to use a temporary regulator to provide for absolute convergence of the integrals. In the following we have used  $\exp(-\beta\hat{H})$  for this purpose—the potentials have been chosen so that this is legitimate.

Since the energy spectrum is bounded from below, we can use this lower bound to give a majorant in the M-test and hence to justify the formula

$$\text{Tr}(\hat{\rho}_\varepsilon \hat{A}) = \lim_{\beta \rightarrow 0^+} \sum_{n,k} \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left[-\frac{1}{2\varepsilon^2}(E_n - E)^2 - \beta E_n\right] \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle, \quad (11)$$

for  $\hat{A} = A(\hat{x})$  as before. The Fourier transform of a Gaussian distribution will now give the integral representation

$$\int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} e^{-\frac{1}{2}\varepsilon^2\alpha^2 + i\alpha E - i\alpha R} = \frac{1}{\sqrt{2\pi\varepsilon^2}} e^{-\frac{1}{2\varepsilon^2}(R-E)^2}, \quad (12)$$

which, by using the bound  $\text{Tr}[\hat{A}|e^{-\beta\hat{H}}] < \infty$  in the Lebesgue dominated convergence theorem, will lead to the result

$$\text{Tr}(\hat{\rho}_\varepsilon \hat{A}) = \lim_{\beta \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} e^{-\frac{1}{2}\varepsilon^2\alpha^2 + i\alpha E} \text{Tr}\left[e^{-(\beta+i\alpha)\hat{H}} \hat{A}\right]. \quad (13)$$

The trace in the integrand of (13) has now a path-integral expression given by (9). Inserting the path-integral formula, referring once more to the dominated convergence theorem to move the “continuum limit” over the  $\alpha$ -integration and applying the Fubini theorem and eq. (12) will then yield

$$\text{Tr}(\hat{\rho}_\varepsilon \hat{A}) = \lim_{\beta} \lim_N \int \frac{d^N x d^N p}{(2\pi)^N} \frac{A(x_0)}{\sqrt{2\pi\varepsilon^2}} \exp\left[i \sum p_k(x_{k-1} - x_k) - \beta\varepsilon S - \frac{1}{2}(S - W)^2\right]. \quad (14)$$

If we now use the equality

$$-\beta\varepsilon S - \frac{1}{2}(S - W)^2 = -\frac{1}{2}(S - W + \beta\varepsilon)^2 + \frac{1}{2}\beta^2\varepsilon^2 - \beta\varepsilon W \quad (15)$$

and take the limit of the last two  $N$ -independent terms, the effect of using the regulator will reduce to a shifting of the energy  $E$  by  $-\beta\varepsilon^2$ . But since the series in (11) clearly converges uniformly in  $E$  and thus gives a continuous function in it, the limit  $\beta \rightarrow 0^+$  will amount to setting  $\beta = 0$  in (14).

Therefore, we have proved that

$$\text{Tr}(\hat{\rho}_\varepsilon \hat{A}) = \lim_{N \rightarrow \infty} \int d^N x A(x_0) K_N(x; E, \varepsilon), \quad (16)$$

where the kernel is given by

$$K_N(x; E, \varepsilon) = \int \frac{d^N p}{(2\pi)^N} \frac{e^{i \sum p_k(x_{k-1} - x_k)}}{\sqrt{2\pi\varepsilon^2}} \exp\left[-\frac{1}{2}\left(\frac{p^2}{2mN\varepsilon} + S_1(x; \varepsilon) - W\right)^2\right]. \quad (17)$$

Most of this integral can be evaluated by choosing spherical coordinates with the  $N$ -axis pointing in the direction of the vector  $(x_{k-1} - x_k)$ . Let us denote by  $y$  the rotated  $N$ -coordinate and let us gather the remaining components into a  $N-1$ -dimensional vector  $q$ . Then the kernel can be rewritten as

$$K_N = \int \frac{d^{N-1} q}{(2\pi)^{N-1}} \int_{-\infty}^{\infty} \frac{dy}{2\pi} \frac{e^{iy\sqrt{\sum_k (x_{k-1} - x_k)^2}}}{\sqrt{2\pi\varepsilon^2}} \exp\left[-\frac{1}{2}\left(\frac{y^2 + q^2}{2mN\varepsilon} + S_1 - W\right)^2\right]. \quad (18)$$

Next we will choose polar coordinates in the  $q$ -space and rescale both  $q$  and  $y$  by the factor  $1/\sqrt{2mN\varepsilon}$ . Since the integrand is independent of the angles and the area of the unit sphere in  $\mathbb{R}^n$  is given by  $2\pi^{n/2}\Gamma(n/2)^{-1}$ , we will then arrive at the formula

$$K_N = \frac{2(mN\varepsilon)^{\frac{N}{2}}}{(2\pi)^{\frac{N}{2}}\Gamma(\frac{N-1}{2})\sqrt{2\pi^2\varepsilon^2}} \int_0^\infty dq q^{N-2} \int_{-\infty}^\infty dy \exp\left[i2y\sqrt{S_0} - \frac{1}{2}(y^2 + q^2 + S_1 - W)^2\right], \quad (19)$$

where we have made use of the definitions in (10).

It is possible to re-express this Fourier transform as a one-dimensional real integral. If we choose polar coordinates in the  $(y, q)$ -plane, utilize the following integral representation for the Bessel functions of the first kind,<sup>9</sup>

$$\int_0^\pi d\theta \sin^{N-2}\theta e^{iv\cos\theta} = \Gamma\left(\frac{N-1}{2}\right) \sqrt{\pi}(2/v)^{\frac{N-2}{2}} J_{\frac{N-2}{2}}(v), \quad (20)$$

and, finally, denote  $r = y^2 + q^2$  and  $\nu = \frac{N-2}{2}$ , we have

$$K_N = \left(\frac{mN\varepsilon}{2\pi}\right)^{\frac{N}{2}} \frac{1}{\sqrt{2\pi\varepsilon^2}} \int_0^\infty dr \left(\frac{r}{S_0}\right)^{\frac{\nu}{2}} J_\nu\left(2\sqrt{S_0 r}\right) \exp\left[-\frac{1}{2}(r + S_1 - W)^2\right]. \quad (21)$$

The integral representation (21) can now be used to derive a series expansion for the kernel. Since

$$\left(\frac{r}{S_0}\right)^{\frac{\nu}{2}} J_\nu\left(2\sqrt{S_0 r}\right) = \sum_{n=0}^\infty \frac{(-S_0)^n r^{\nu+n}}{n! \Gamma(\nu + n + 1)}, \quad (22)$$

the expansion of the exponential  $\exp[-r(S_1 - W)]$  and a subsequent term by term integration will give

$$K_N = \left(\frac{mN\varepsilon}{2\pi}\right)^{\frac{N}{2}} \frac{\exp\left[-\frac{1}{2}(S_1 - W)^2\right]}{\sqrt{2\pi\varepsilon^2}} \sum_{n=0}^\infty \sum_{k=0}^n \frac{(-S_0)^k}{k!} \frac{(W - S_1)^{n-k}}{(n-k)!} \frac{2^{\frac{\nu-1+n}{2}} \Gamma\left(\frac{\nu+1+n}{2}\right)}{\Gamma(\nu + 1 + k)}, \quad (23)$$

which, however, has no immediate applications for evaluation of the kernel, because the convergence of the sum will be too slow for large values of the parameters.

So far, the best way to evaluate the kernel  $K_N$  for large enough range of parameter values has been a numerical integration of eq. (21). This is mainly due to the well-developed methods of computation of the values of the Bessel functions. Similar methods—recursion relations, integral representations, etc.—will likely offer more efficient ways of evaluating the kernel as well. However, since the numerical integration was sufficiently fast for our purposes, we do not pursue this point further here.

#### IV. NUMERICAL EVALUATION OF THE LATTICE EXPECTATION VALUES

The purpose of this section is to enable a Monte Carlo integration of the lattice expectation values in (16). From the experience in the lattice quantum field simulations, this

should be possible provided that the following condition is met: the Monte Carlo is used for a generation of a probability distribution  $\exp(-S[x])$ , where  $S[x]$  is a *local* action. The locality, which means that the action is a sum over a local “action density”, makes it possible to use local updating algorithms and in this way to achieve a fast enough generation of the required probability distribution. In the following we will derive an exponential bound for the kernel, but with an “action”, which is not local. However, as explained at the end of this section, a certain linear approximation for the exponent will be a local quantity, using which it is still possible to benefit from the local updating algorithms.

Letting  $r = q^2$  in (19) will give the starting point for the approximations:

$$K_N = \frac{(mN\varepsilon)^{\frac{N}{2}}}{(2\pi)^{\frac{N}{2}}\Gamma(\frac{N-1}{2})\sqrt{2\pi^2\varepsilon^2}} \int_0^\infty dr r^{\frac{N-3}{2}} \int_{-\infty}^\infty dy \exp\left[i2y\sqrt{S_0} - \frac{1}{2}(y^2 + r + S_1 - W)^2\right]. \quad (24)$$

Next we need to rely on the lemmas proved in the Appendix. First on Lemma A.1, which states that for all real  $\lambda$ , the  $y$  in the integrand of (24) can be replaced by  $y+i\lambda$ , i.e. that the double integral is always equal to

$$\int_0^\infty dr r^{\frac{N-3}{2}} \int_{-\infty}^\infty dy \exp\left[i2y\sqrt{S_0} - 2\lambda\sqrt{S_0} - \frac{1}{2}(y^2 - \lambda^2 + r + S_1 - W + i2\lambda y)^2\right]. \quad (25)$$

The absolute value of this quantity is less than

$$\int_{-\infty}^\infty dy \exp\left[-2\lambda\sqrt{S_0} + 2\lambda^2 y^2\right] \int_0^\infty dr r^{\frac{N-3}{2}} \exp\left[-\frac{1}{2}(r + y^2 - \lambda^2 + S_1 - W)^2\right]. \quad (26)$$

Now we are ready to apply Lemma A.2 to get an upper bound for the second integral,

$$\int_{-\infty}^\infty dy \exp\left[-2\lambda\sqrt{S_0} + 2\lambda^2 y^2\right] \frac{\sqrt{\pi}\Gamma(\frac{N-1}{2})}{2^{\frac{N-1}{4}}\Gamma(\frac{N+1}{4})} \exp\left[-b_N(y^2 - \lambda^2 + S_1 - W)\right], \quad (27)$$

with  $b_N = \sqrt{2}\Gamma(\frac{N+1}{4})/\Gamma(\frac{N-1}{4})$  (for large values of  $N$ ,  $b_N$  can be approximated by  $\sqrt{\frac{N-2}{2}} = \sqrt{\nu}$ ). Since

$$\int_{-\infty}^\infty dy \exp\left[-(b_N - 2\lambda^2)y^2\right] = \sqrt{\frac{\pi}{b_N - 2\lambda^2}} \leq \sqrt{\pi}, \quad (28)$$

whenever  $2\lambda^2 \leq b_N - 1$ , we can infer from (27) that for these values of  $\lambda$

$$|K_N| \leq \left(\frac{mN\varepsilon}{2\pi}\right)^{\frac{N}{2}} \frac{1}{\sqrt{2\pi\varepsilon^2}} \frac{\sqrt{\pi}}{2^{\frac{N-1}{4}}\Gamma(\frac{N+1}{4})} \exp\left[-2\lambda\sqrt{S_0} + b_N\lambda^2 - b_N(S_1 - W)\right]. \quad (29)$$

As a function of  $\lambda$ , the right hand side has only one minimum which lies at  $\lambda = \sqrt{S_0}/b_N$ . If  $S_0 \leq b_N^2(b_N - 1)/2$ , we can use this value of  $\lambda$  to give the upper bound, and the exponential factor will become  $\exp[-S_0/b_N - b_N(S_1 - W)]$ .

Let us now use notation  $M_N$  for the critical value of  $S_0$ —for large  $N$ ,  $M_N$  is approximately equal to  $\sqrt{\nu^3}/2$ . If  $S_0 > M_N$ , the best allowed value is then given by  $\lambda = \sqrt{\frac{b_N-1}{2}} = \sqrt{M_N}/b_N$ , which yields the exponential factor  $\exp[-(2\sqrt{M_N S_0} - M_N)/b_N - b_N(S_1 - W)]$ .

To summarize, we have now proved that

$$|K_N| \leq \left(\frac{mN\varepsilon}{2\pi}\right)^{\frac{N}{2}} \frac{1}{\sqrt{2\pi\varepsilon^2}} \frac{\sqrt{\pi}}{2^{\frac{N-1}{4}}\Gamma(\frac{N+1}{4})} \exp\left[Wb_N - \left(\frac{S_0}{b_N} + b_N S_1\right)\right] \times \exp\left[\Theta(S_0 - M_N) \frac{(\sqrt{S_0} - \sqrt{M_N})^2}{b_N}\right], \quad (30)$$

where  $\Theta$  denotes the step function. As a curiosity, it should be noted that the term  $S_0/b_N + b_N S_1$  corresponds to a certain “renormalized” finite temperature lattice action—renormalized in the sense that the temperature of the action depends on the size of the lattice:  $T(N) = \varepsilon/b_N$ .

We propose that the lattice ensemble expectation values could be evaluated by using a Monte Carlo sampling to generate a distribution  $\exp(-S^{(N)}(x; E, \varepsilon))$  and thus allowing the evaluation of the ratios<sup>10</sup>

$$\frac{\int d^N x A(x_0) \tilde{K}_N(x; E, \varepsilon) \exp(-S^{(N)}(x; E, \varepsilon))}{\int d^N x \tilde{K}_N(x; E, \varepsilon) \exp(-S^{(N)}(x; E, \varepsilon))}, \quad (31)$$

where  $\tilde{K}_N$  is obtained from the scaling of the kernel by the inverse of the right hand side of (30) and the “lattice action”  $S^{(N)}$  is given by the formula

$$S^{(N)} = \frac{S_0 - \Theta(S_0 - M_N) (\sqrt{S_0} - \sqrt{M_N})^2}{b_N} + b_N (S_1 - E/\varepsilon). \quad (32)$$

For local updating algorithms, the value of the action could be computed exactly at the beginning of each sweep and the linear approximation

$$\Delta S^{(N)} = \frac{c}{b_N} \Delta S_0 + b_N \Delta S_1 \quad (33)$$

could be used during the sweep. In the linear approximation,  $c = 1$ , if  $S_0 \leq M_N$  at the beginning of the sweep, and  $c = \sqrt{M_N/S_0}$  otherwise.

To check that the approximations used in the derivation of the upper bound are reasonable, we have shown a plot of values of the normalized kernel  $\tilde{K}_N$  with  $N = 22$  and  $W = 7$  in Fig. 1. Two general features are evident from the figure: firstly, there is a “gaussian wall” around the line  $S_1 = W$ , which means that the importance sampling should extend at least that far in the  $S_1$ -direction. Secondly, although the scaling can be seen to be quite optimal for the region  $S_0 \leq M_N$ , the scaled values drop rapidly after that point. The oscillations of the kernel, however, also begin at about the same values of  $S_0$  and an oversampling of the oscillatory region is in fact only desirable—therefore, the use of this particular scaling function is qualitatively justified.



## V. CONCLUSIONS

We have defined a Gaussian quantum statistical ensemble for the approximation of micro-canonical expectation values of any system which is amenable for the usual Gibbs ensemble treatment. We have also derived a method for the computation of these expectation values by a Monte Carlo integration on a time-lattice, provided that the Hamiltonian allows an analytic lattice regularization. The generalization of these results for quantum field theories and tests for the numerical efficiency of the lattice approximation are currently under investigation.

## ACKNOWLEDGMENTS

I would like to thank Masud Chaichian, Antti Kupiainen, Claus Montonen and Esko Suhonen for their scientific guidance and support and Sami Virtanen for several useful discussions.

## APPENDIX A:

In this Appendix we shall prove the two lemmas that were used in Section IV to derive the exponential bound for the integral kernel.

**Lemma A.1** *Let  $f$  be defined by the formula  $f(y) = \exp[iby - \frac{1}{2}(y^2 + C)^2]$ , where  $C$  and  $b$  are complex parameters. The integrals of  $f$  over lines parallel to the real axis are all equal:*

$$\int_{-\infty}^{\infty} dy f(y + i\lambda) = \int_{-\infty}^{\infty} dy f(y), \text{ for all } \lambda \in \mathbb{R}.$$

**Proof.** Consider the integral of  $f$  over a contour following the perimeter of a square with corners at points  $\pm R, \pm R + i\lambda$ . Since  $f$  is a composition of two entire functions, it is entire and the integral over this contour is therefore zero by the Cauchy theorem. Writing this integral in a parameter form gives

$$\int_{-R}^R dy f(y) = \int_{-R}^R dy f(y + i\lambda) - i\lambda \int_0^1 dt (f(R + i\lambda t) - f(-R + i\lambda t)).$$

But since for all  $0 \leq t \leq 1$ ,

$$|f(\pm R + i\lambda t)| \leq \exp \left[ |bR| + |b\lambda| - \frac{1}{2}(R^2 - \lambda^2 - |C|)^2 + \frac{1}{2}(2|\lambda| + |C|)^2 \right],$$

and the upper bound goes to zero when  $R$  goes to infinity, the integral over  $t$  vanishes when we take the limit  $R \rightarrow \infty$  and the lemma follows.  $\square$

**Lemma A.2** For all  $\tau > 0$  and  $C \in \mathbb{R}$

$$\int_0^\infty dr r^\tau e^{-\frac{1}{2}(r+C)^2} \leq a_\tau e^{-b_\tau C},$$

where  $a_\tau$  and  $b_\tau$  are positive constants given by the formulae

$$a_\tau = \frac{\sqrt{\pi}\Gamma(\tau+1)}{2^{\frac{\tau+1}{2}}\Gamma(\frac{\tau+2}{2})}, \quad b_\tau = \frac{\sqrt{2}\Gamma(\frac{\tau+2}{2})}{\Gamma(\frac{\tau+1}{2})}.$$

**Proof.** Let us use the notation  $I_\tau(C)$  for the integral  $\int_0^\infty dr r^\tau e^{-\frac{1}{2}(r+C)^2}$ . The integral converges for  $\tau > -1$ , when  $I_\tau$  defines a function from the real numbers to  $(0, \infty)$ . We claim that the following three properties are satisfied for all  $C$ , if  $\tau > 0$ :

- (a)  $I_{\tau+1}(C) = \tau I_{\tau-1}(C) - C I_\tau(C)$ ,
- (b)  $I_\tau$  is differentiable at  $C$  and  $I'_\tau(C) = -I_{\tau+1}(C) - C I_\tau(C) = -\tau I_{\tau-1}(C)$ ,
- (c)  $\frac{I_{\tau+1}(C)}{I_\tau(C)} > \frac{I_\tau(C)}{I_{\tau-1}(C)}$ .

The lemma is then a fairly straightforward consequence of these results.

Fix  $\tau > 0$  and define  $g(C) = \ln I_\tau(C)$ . Applying (b) twice shows that the first and the second derivatives of  $g$  exist and that they are  $g' = -\tau I_{\tau-1}/I_\tau$  and  $g'' = -\tau(\frac{I_{\tau+1}}{I_\tau} - 1)$ . But from (c) we now deduce that  $g'' < 0$  and therefore  $g$  is a concave differentiable function. This means that every tangent line to  $g$  is an upper bound for the function: for every fixed  $D \in \mathbb{R}$ ,  $g(C) \leq (C - D)g'(D) + g(D)$ . Exponentiation of both sides of this inequality gives now

$$I_\tau(C) \leq I_\tau(D) \exp\left[-\tau \frac{I_{\tau-1}(D)}{I_\tau(D)}(C - D)\right],$$

which is of the desired form if we just define  $b_\tau = \tau I_{\tau-1}(D)/I_\tau(D)$  and  $a_\tau = I_\tau(D) \exp[b_\tau D]$ .

It now remains to show that the explicit formulas given in the Lemma for  $a_\tau$  and  $b_\tau$  are valid for some  $D$ . Choose  $D = 0$ , when a change of variables from  $r$  to  $\frac{1}{2}r^2$  shows that  $I_\tau(0) = 2^{\frac{\tau+1}{2}}\Gamma(\frac{\tau+1}{2})$ . On the other hand, an application of (a) reveals that for  $D = 0$ ,  $b_\tau = I_{\tau+1}(0)/I_\tau(0)$ , which then simplifies into the desired formula. Since now  $a_\tau = I_\tau(0)$ , the form for  $a_\tau$  is a consequence of the Gamma-function “doubling formula”:  $\Gamma(\frac{z}{2})\Gamma(\frac{z+1}{2}) = 2^{1-z}\Gamma(\frac{1}{2})\Gamma(z)$ .

Therefore, it is necessary only to show that the propositions (a)–(c) hold. (a) is obtained by a simple partial integration, since  $r \exp[-\frac{1}{2}(r+C)^2] = -\frac{d}{dr} \exp[-\frac{1}{2}(r+C)^2] - C \exp[-\frac{1}{2}(r+C)^2]$  and the boundary terms vanish for  $\tau > 0$ .

Consider next the finite difference term,  $I_\tau(C + h) - I_\tau(C)$ . This is equal to  $\int_0^\infty dr r^\tau e^{-\frac{1}{2}(r+C)^2} \{\exp[-\frac{1}{2}h^2 - h(r+C)] - 1\}$ , where the term in the braces is bounded by  $\exp[|h|r + |hC|] + 1$ . Lebesgue dominated convergence theorem now shows that it is possible to differentiate under the integral sign, which will prove the differentiability and the first equality in (b). The second equality follows then by an application of (a).

To prove (c), it is enough to show that  $I_{\tau+1}(C)I_{\tau-1}(C) - I_\tau^2(C) > 0$ , for all  $C$  and  $\tau > 0$ . Expressing the products as two-dimensional integrals will yield

$$I_{\tau+1}(C)I_{\tau-1}(C) - I_{\tau}^2(C) = \int_0^{\infty} dx \int_0^{\infty} dy x^{\tau} y^{\tau-1} (x-y) \exp \left[ -\frac{1}{2} ((x+C)^2 + (y+C)^2) \right].$$

In the change of variables  $(x, y) \rightarrow (t, u) = (x + y, \frac{x-y}{x+y})$ , the Jacobian equals  $\frac{1}{2}t$  and the integration region changes into  $(0, \infty) \times (-1, 1)$ . This way the integral becomes

$$\int_0^{\infty} dt \int_{-1}^1 du 2^{-2\tau} t^{2\tau+1} (u+u^2)(1-u^2)^{\tau-1} \exp \left[ -\frac{1}{4} t^2 (1+u^2) - Ct - C^2 \right].$$

As the region of integration over  $u$  is symmetric, the antisymmetric part vanishes, and we arrive at the result

$$I_{\tau+1}(C)I_{\tau-1}(C) - I_{\tau}^2(C) = \int_0^{\infty} dt \int_{-1}^1 du 2^{-2\tau} t^{2\tau+1} u^2 (1-u^2)^{\tau-1} \exp \left[ -\frac{1}{4} t^2 (1+u^2) - Ct - C^2 \right],$$

which is always strictly positive.  $\square$

<sup>1</sup> K. Redlich, J. Cleymans, H. Satz and E. Suhonen, Nucl. Phys. **A 566**, 391c (1994)

<sup>2</sup> P. Braun-Munzinger, J. Stachel, J. P. Wessels and N. Xu, Phys. Lett. **B 365**, 1 (1996)

<sup>3</sup> M. Chaichian and I. Senda, Nucl. Phys. **B 396**, 737 (1993)

<sup>4</sup> M. Chaichian, H. Satz and I. Senda, Phys. Rev. **D 49**, 1566 (1994)

<sup>5</sup> On physical grounds, the idea of using a Gaussian energy distribution to define a statistical ensemble seems natural. Such a physical reasoning was adopted, for instance, in J. H. Hetherington and D. R. Stump, Phys. Rev. **D 35**, 1972 (1987), to introduce a Gaussian ensemble for studying first order phase transitions in certain lattice gauge theories.

<sup>6</sup> M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness* (Academic Press, New York, 1975). The essential self-adjointness follows from Theorem X.32 and a derivation of the Feynman-Kac kernel is given in Section X.11.

<sup>7</sup> B. Simon, *Functional Integration and Quantum Physics* (Academic Press, New York, 1979). Theorem 9.2. and its proof explain the trace-class statement.

<sup>8</sup> It is fairly easy to prove that the left hand side of (9) is an analytic function in the region  $\text{Re } \beta > 0$ , if  $V$  is a polynomial bounded from below. If we also assume that  $A$  is a polynomial, the analyticity of the right hand side will follow from an application of the Cauchy theorem, but only in the sector  $|\text{Arg } \beta| < \frac{\pi}{n+2}$ , where  $n$  is the degree of  $V$ .

<sup>9</sup> I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1980), 4th ed., formula 3.915.5.

<sup>10</sup> Note that all  $x$ -independent scaling factors, coming from the normalization of the probability distribution  $\exp(-S^{(N)})$ , vanish in the ratio.

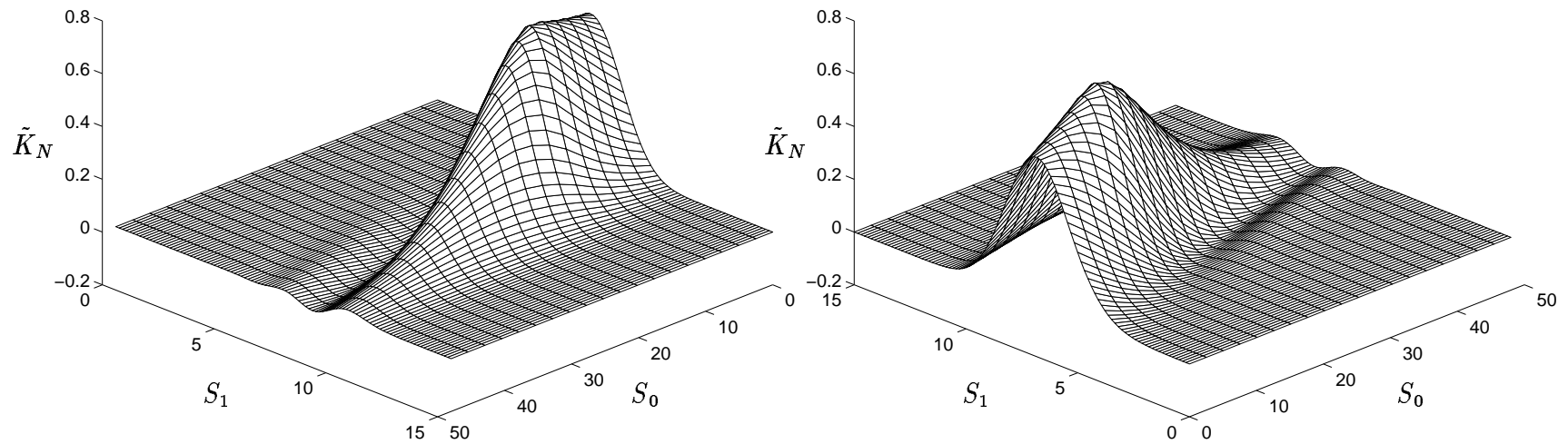


FIG. 1. Values of the normalized kernel  $\tilde{K}_N$  as a function of the variables  $S_0$  and  $S_1$  from two different viewpoints. Here  $W = E/\varepsilon = 7$  and  $N = 22$ , which corresponds to  $\nu = 10$ ,  $b_N \approx 3.24$  and  $M_N \approx 11.8$ . The maximum value at the peak near  $S_0 = M_N$ ,  $S_1 = W$  is approximately 0.67.